chain nodes :
     7   8   9   10   17
ring nodes :
     1   2   3   4   5   6   11   12   13   14   15   16
chain bonds :
     5-7   7-8   8-9   9-10   10-12   13-17
ring bonds :
     1-2   1-6   2-3   3-4   4-5   5-6   11-12   11-16   12-13   13-14   14-15   15-16
exact/norm bonds :
     5-7   7-8   8-9   9-10   10-12   11-12   11-16   12-13   13-14   13-17   14-15   15-16
normalized bonds :
     1-2   1-6   2-3   3-4   4-5   5-6
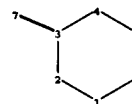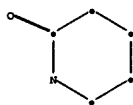isolated ring systems :
     containing 11 :

G1:O,S,N,CH2

Match level :
     1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS   10:CLASS
     11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   16:Atom   17:CLASS

chain nodes :
    7
ring nodes :
    1   2   3   4   5   6
chain bonds :
    3-7
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6
exact/norm bonds :
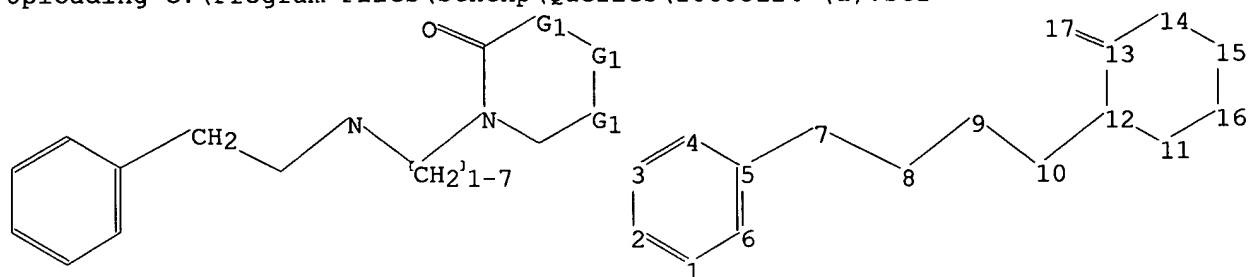   1-2   1-6   2-3   3-4   3-7   4-5   5-6

G1:O,S,N,CH2

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS

=>
Uploading C:\Program Files\Stnexp\Queries\10685124 (a).str

chain nodes :
7 8 9 10 17
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 16
chain bonds :
5-7 7-8 8-9 9-10 10-12 13-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
exact/norm bonds :
5-7 7-8 8-9 9-10 10-12 11-12 11-16 12-13 13-14 13-17 14-15 15-16
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 11 :

G1:O,S,N,CH2

Match level :
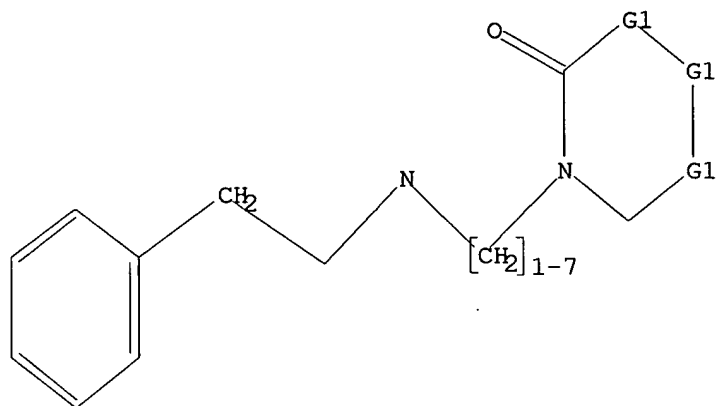1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR

G1 O,S,N,CH2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss sam
SAMPLE SEARCH INITIATED 14:28:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     1457 TO ITERATE

100.0% PROCESSED     1457 ITERATIONS                          8 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   **COMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:         26851 TO      31429
PROJECTED ANSWERS:                8 TO        329

L2            8 SEA SSS SAM L1

=> => s l1 sss ful
FULL SEARCH INITIATED 14:28:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    29039 TO ITERATE

100.0% PROCESSED    29039 ITERATIONS                        173 ANSWERS
SEARCH TIME: 00.00.01

L3           173 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10685124 (sub).str
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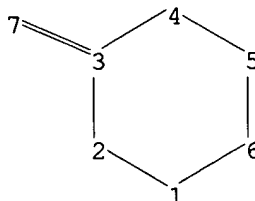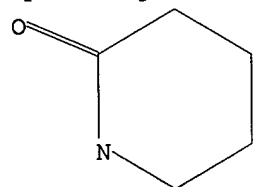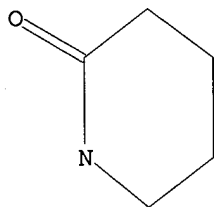

chain nodes :

7
ring nodes :
1 2 3 4 5 6
chain bonds :
3-7
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 3-7 4-5 5-6

G1:O,S,N,CH2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS

L4   STRUCTURE UPLOADED

=> d 14
L4 HAS NO ANSWERS
L4   STR

G1 O,S,N,CH2

Structure attributes must be viewed using STN Express query preparation.

=> s 14 sub=13 sss sam
SAMPLE SUBSET SEARCH INITIATED 14:29:52 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -   6 TO ITERATE

100.0% PROCESSED   6 ITERATIONS   6 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):   ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):   6 TO   266
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):   6 TO   266

L5   6 SEA SUB=L3 SSS SAM L4

=> => s 14 sub=13 sss ful
FULL SUBSET SEARCH INITIATED 14:30:16 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -   98 TO ITERATE

100.0% PROCESSED   98 ITERATIONS   90 ANSWERS
SEARCH TIME: 00.00.01

```
L6               90 SEA SUB=L3 SSS FUL L4

=> s l3 not l6
L7               83 L3 NOT L6

=> => s l7
L8                2 L7

=> d l8 1-2 bib,ab,hitstr
```

```
L8    ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2005 ACS on STN
AN    2001:868427  CAPLUS
DN    136:6016
TI    Preparation of aminoalkyllactams as muscarinic receptor antagonists
IN    Dvorak, Charles Alois; Fisher, Lawrence Emerson; Green, Keena Lynn;
      Harris, Ralph New, III; Maag, Hans; Prince, Anthony; Repke, David Bruce;
      Stabler, Russell Stephen
PA    F. Hoffmann-La Roche A.-G., Switz.
SO    PCT Int. Appl., 100 pp.
      CODEN: PIXXD2
DT    Patent
LA    English
FAN.CNT 2
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Appl PCT

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        PATENT NO.              KIND   DATE        APPLICATION NO.           DATE
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PI  WO 2001090081               A1     20011129    WO 2001-EP5584            20010516
    W:  AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CU,
        CZ, DE, DK, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
        IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
        MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
        SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY,
        KG, KZ, MD, RU, TJ, TM
    RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
        DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
        BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    CA 2409841                                    CA 2001-2409841           20010516
    EP 1289965                  AA     20011129    EP 2001-980030            20010516
    R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
        IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
    BR 2001011061               A1     20030312
    JP 2003534330               A      20030415    BR 2001-11061
    NZ 522411                   T2     20031118    JP 2001-586270            20010516
    RU 2241702                  A      20040528    NZ 2001-522411            20010516
    AU 782191                   C2     20041210    RU 2002-133208            20010516
    US 2002004501               B2     20050707    AU 2002-10122             20010516
    US 6667301                  A1     20020110    US 2001-862286            20010516
    ZA 2002008895               B2     20031223                              20010522
    US 2003109524               A      20040219
    US 6645958                  A1     20030612    ZA 2002-8895
    ZA 2002009029               B2     20031111    US 2002-289055            20021101
    NO 2002005640               A      20040206                              20021106
    US 2004034018               A      20030122    ZA 2002-9029
    US 6818645                  A1     20040219    NO 2002-5640              20021106
    US 2004087581               B2     20041116    US 2003-632734            20021122
PRAI US 2000-207483P            A1     20040506                              20030801
    US 2001-267579P             P      20000525    US 2003-685124            20031014
    US 2001-267617P             P      20010209
    WO 2001-EP5584              P      20010209
    US 2001-862286              W      20010516
    US 2001-862522              A3     20010522
    US 2002-289055              A3     20010522
OS  MARPAT 136:6016             A3     20021106
```

AB Preparation of aminoalkyllactams (I) (one of X, Y or Z = independently -S-,-O-,
    CH2- or >N-R6, the others are -CH2-; m = 0-3; n = 1-6; R4 = alkyl; R5 =
    alkyl, alkenyl, alkynyl or cycloalkyl; and R1, R2, and R3 = H or specified
    substituents). Thus, I (R1 = 4-MeO; R2, R3 = H; R4 = Me; R5 = Et; n = 1;
    m = 0; X, Y, Z = CH2) (II) is prepared by reaction of (2-oxo-
    pyrrolidinyl)acetaldehyde with [2-(4-methoxyphenyl)-1-

methyethyl]ethylamine and sodium triacetoxyborohydride in
1,2-dichloroethane. II shows pKi of 7.32, 6.95 and 5.36 in muscarinic
(M2, M3, M5) inhibitory activity against hamster ovary cells. I are
generally muscarinic M2/M3 receptor antagonists and formulations are given
for treating diseases associated with smooth muscle disorders.

IT   **376577-81-0P 376577-86-5P 376577-90-1P**
        376577-92-3P 376577-94-5P 376577-96-7P
        376577-97-8P 376577-98-9P 376577-99-0P
        376578-00-6P 376578-03-9P 376578-04-0P
        376578-12-0P 376578-13-1P 376578-14-2P
        376578-15-3P 376578-21-1P 376578-23-3P
        376578-24-4P 376578-25-5P 376578-63-1P
        376578-64-2P 376578-66-4P 376578-67-5P
        376578-69-7P 376578-74-4P 376578-75-5P
        376578-78-8P 376578-82-4P 376579-69-0P
        376579-71-4P 376579-73-6P 376579-75-8P
        376579-77-0P 376579-79-2P 376579-81-6P
        376579-83-8P 376579-85-0P 376579-87-2P
        376579-89-4P 376579-91-8P

    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
    (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
    (Uses)
       (preparation of aminoalkyllactams as muscarinic receptor antagonists)

RN   376577-81-0 CAPLUS
CN   2H-1,3-Oxazin-2-one, 3-[4-[ethyl[(1S)-1-methyl-2-[4-
    (methylsulfonyl)phenyl]ethyl]amino]butyl]tetrahydro-, monohydrochloride
    (9CI) (CA INDEX NAME)

Absolute stereochemistry.
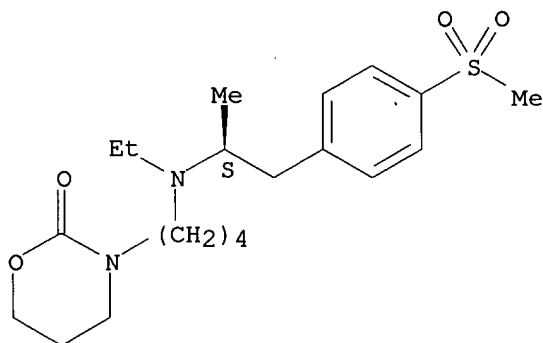
● HCl

RN   376577-86-5 CAPLUS
CN   2H-1,3-Oxazin-2-one, 3-[4-[ethyl[1-methyl-2-[4-
    [(trifluoromethyl)sulfonyl]phenyl]ethyl]amino]butyl]tetrahydro-,
    monohydrochloride (9CI) (CA INDEX NAME)

F3C—S(=O)(=O)— [benzene ring] —CH2—CH(Me)—N(Et)—(CH2)4—[N, tetrahydro-1,3-thiazin-2-one ring with O, S]
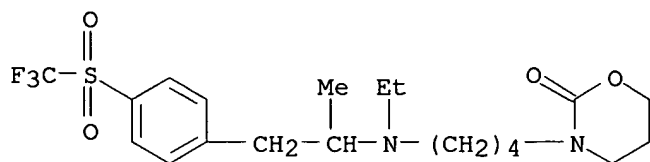
● HCl

RN   376577-90-1 CAPLUS
CN   2H-1,3-Thiazin-2-one, 3-[4-[ethyl[1-methyl-2-[4-
      (methylsulfonyl)phenyl]ethyl]amino]butyl]tetrahydro-, monohydrochloride
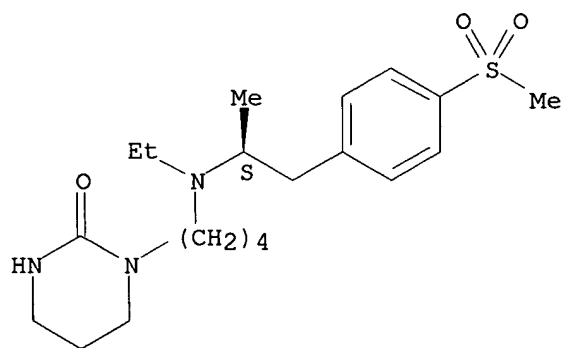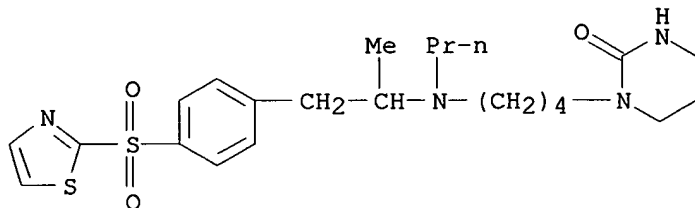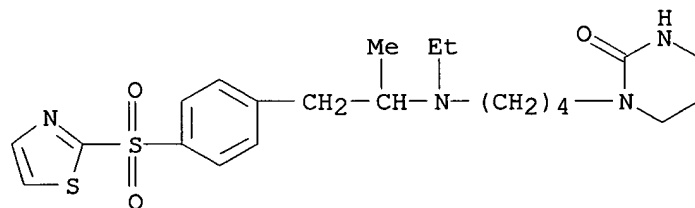   (9CI) (CA INDEX NAME)

Me—S(=O)(=O)— [benzene ring] —CH2—CH(Me)—N(Et)—(CH2)4—[N, tetrahydro-1,3-thiazin-2-one ring with O, S]
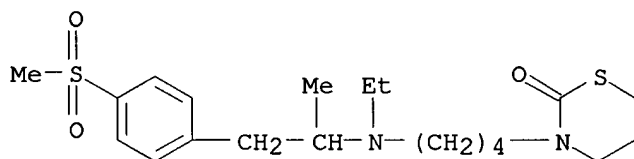
● HCl

RN   376577-92-3 CAPLUS
CN   Butanedioic acid, 2,3-bis(benzoyloxy)-, (2R,3R)-, compd. with
      1-[4-[ethyl[2-(4-methoxyphenyl)-1-methylethyl]amino]butyl]tetrahydro-2(1H)-
      pyrimidinone (1:1) (9CI) (CA INDEX NAME)

      CM   1

      CRN   376577-91-2
      CMF   C20 H33 N3 O2

MeO— [benzene ring] —CH2—CH(Me)—N(Et)—(CH2)4—[N, tetrahydro-2(1H)-pyrimidinone ring with O, NH]

      CM   2
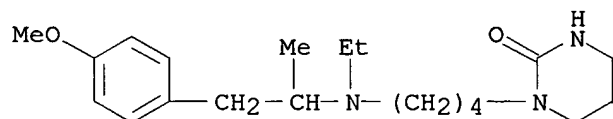
      CRN   2743-38-6
      CMF   C18 H14 O8

Absolute stereochemistry. Rotation (-).
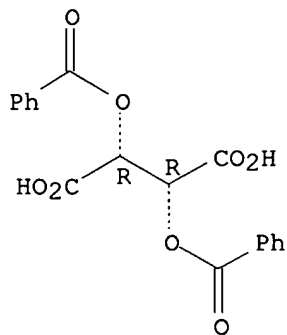
RN   376577-94-5 CAPLUS
CN   Butanedioic acid, 2,3-bis(benzoyloxy)-, (2R,3R)-, compd. with
      1-[4-[ethyl[2-(4-methoxyphenyl)-1-methylethyl]amino]butyl]tetrahydro-3-
      methyl-2(1H)-pyrimidinone (1:1) (9CI)   (CA INDEX NAME)

      CM   1

      CRN   376577-93-4
      CMF   C21 H35 N3 O2

      CM   2
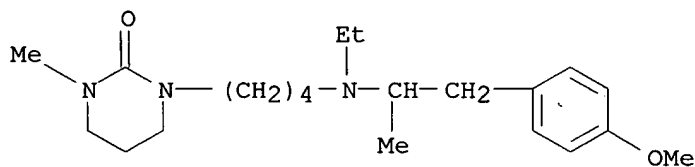
      CRN   2743-38-6
      CMF   C18 H14 O8

Absolute stereochemistry.   Rotation (-).
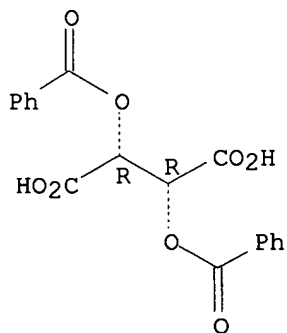
RN   376577-96-7 CAPLUS
CN   Butanedioic acid, 2,3-bis(benzoyloxy)-, (2R,3R)-, compd. with

NAME)

● HCl

RN   376577-99-0   CAPLUS
CN   2(1H)-Pyrimidinone, 1-[3-[[2-(4-chlorophenyl)-1-
      methylethyl]propylamino]propyl]tetrahydro-, monohydrochloride (9CI)   (CA
      INDEX NAME)
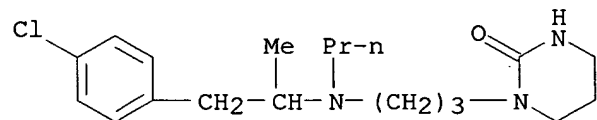
● HCl

RN   376578-00-6   CAPLUS
CN   2(1H)-Pyrimidinone, 1-[4-[ethyl[(1S)-1-methyl-2-[4-
      (methylsulfonyl)phenyl]ethyl]amino]butyl]tetrahydro-, monohydrochloride
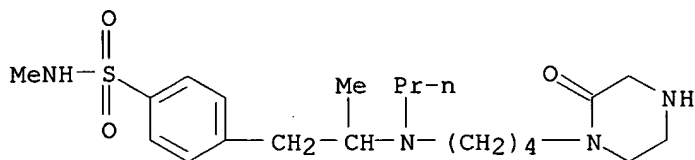   (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN   376578-03-9   CAPLUS
CN   2(1H)-Pyrimidinone, tetrahydro-1-[4-[[1-methyl-2-[4-(2-
      thiazolylsulfonyl)phenyl]ethyl]propylamino]butyl]-, monohydrochloride
      (9CI)   (CA INDEX NAME)

Me Pr-n

CH2—CH—N—(CH2)4—

● HCl

RN   376578-04-0   CAPLUS
CN   2(1H)-Pyrimidinone, 1-[4-[ethyl[1-methyl-2-[4-(2-
      thiazolylsulfonyl)phenyl]ethyl]amino]butyl]tetrahydro-, monohydrochloride
      (9CI)   (CA INDEX NAME)

Me Et

CH2—CH—N—(CH2)4—

● HCl

RN   376578-12-0   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-[(trifluoromethyl)sulfonyl]phenyl]
      ethyl]amino]butyl]-, monohydrochloride (9CI)   (CA INDEX NAME)

F3C—S

Me Et

CH2—CH—N—(CH2)4—N
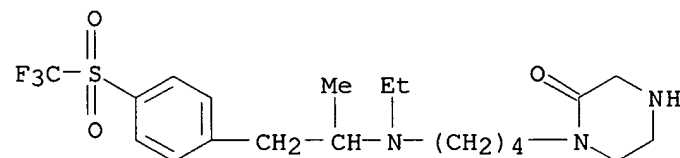
● HCl

RN   376578-13-1   CAPLUS

CN   Benzenesulfonamide, N-methyl-4-[2-[[4-(2-oxo-1-
     piperazinyl)butyl]propylamino]propyl]-, monohydrochloride (9CI)   (CA INDEX
     NAME)

MeNH—S(=O)(=O)—C₆H₄—CH₂—CH(Me)—N(Pr-n)—(CH₂)₄—N(piperazinone)

● HCl

RN   376578-14-2   CAPLUS
CN   Piperazinone, 1-[4-[[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]propylamin
     o]butyl]-, monohydrochloride (9CI)   (CA INDEX NAME)

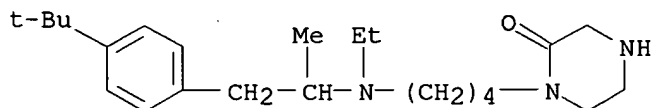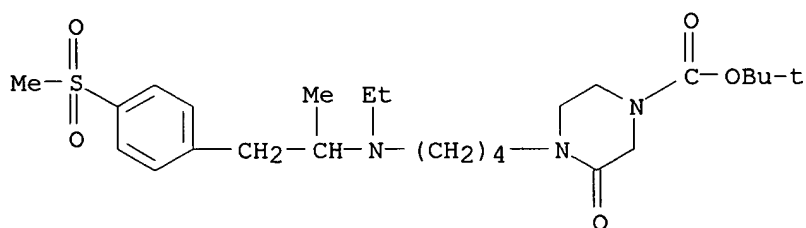Me—S(=O)(=O)—C₆H₄—CH₂—CH(Me)—N(Pr-n)—(CH₂)₄—N(piperazinone)
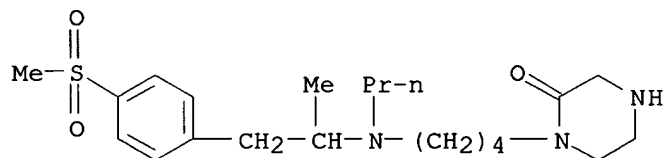
● HCl

RN   376578-15-3   CAPLUS
CN   Piperazinone, 1-[4-[[1-methyl-2-[4-(2-thiazolylsulfonyl)phenyl]ethyl]propy
     lamino]butyl]-, monohydrochloride (9CI)   (CA INDEX NAME)

thiazolyl—S(=O)(=O)—C₆H₄—CH₂—CH(Me)—N(Pr-n)—(CH₂)₄—N(piperazinone)
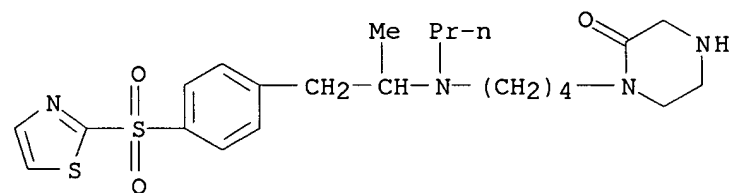
● HCl

RN   376578-21-1   CAPLUS
CN   Piperazinone, 1-[4-[[2-[4-(1,1-dimethylethyl)phenyl]-1-
     methylethyl]ethylamino]butyl]-, monohydrochloride (9CI)   (CA INDEX NAME)

t-Bu—⟨phenyl⟩—CH2—CH(Me)—N(Et)—(CH2)4—N⟨piperazinone⟩NH (with C=O)

● HCl

RN   376578-23-3   CAPLUS
CN   1-Piperazinecarboxylic acid, 4-[4-[ethyl[1-methyl-2-[4-
      (methylsulfonyl)phenyl]ethyl]amino]butyl]-3-oxo-, 1,1-dimethylethyl ester
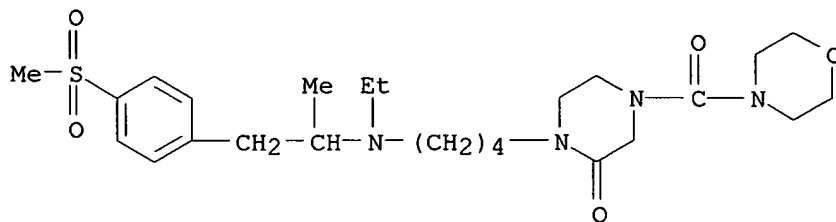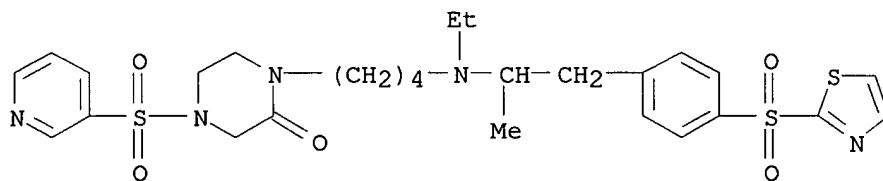   (9CI)   (CA INDEX NAME)

Me—S(O)(O)—⟨phenyl⟩—CH2—CH(Me)—N(Et)—(CH2)4—N⟨piperazinone⟩N—C(O)—OBu-t (with C=O)

RN   376578-24-4   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
      ]butyl]-4-(methylsulfonyl)-, monohydrochloride (9CI)   (CA INDEX NAME)

Me—S(O)(O)—⟨phenyl⟩—CH2—CH(Me)—N(Et)—(CH2)4—N⟨piperazinone⟩N—S(O)(O)—Me (with C=O)
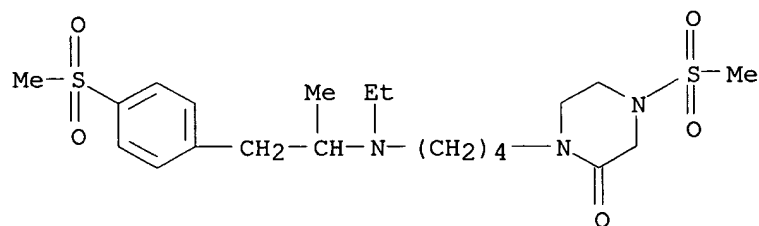
● HCl

RN   376578-25-5   CAPLUS
CN   Morpholine, 4-[[4-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]ami
      no]butyl]-3-oxo-1-piperazinyl]carbonyl]-, monohydrochloride (9CI)   (CA
      INDEX NAME)

● HCl

RN 376578-63-1 CAPLUS
CN Piperazinone, 4-methyl-1-[4-[[1-methyl-2-[4-(2-thiazolylsulfonyl)phenyl]ethyl]propylamino]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)
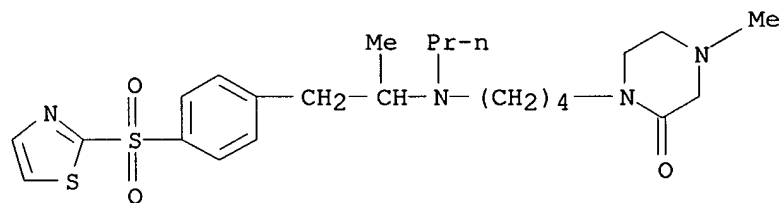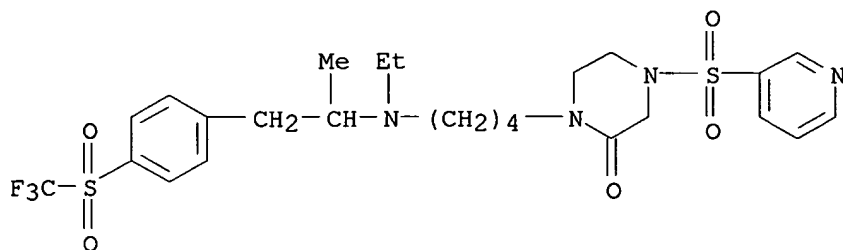

● HCl

RN 376578-64-2 CAPLUS
CN Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(2-thiazolylsulfonyl)phenyl]ethyl]amino]butyl]-4-(3-pyridinylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)
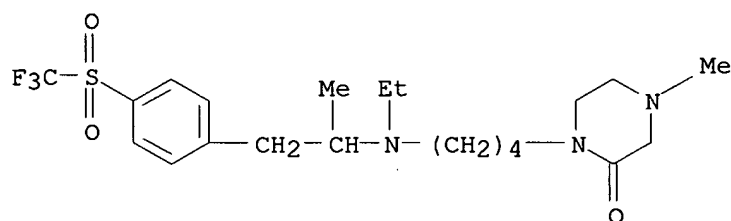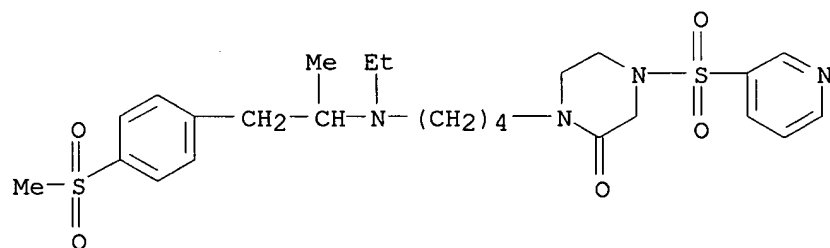

● HCl

RN 376578-66-4 CAPLUS
CN Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-[(trifluoromethyl)sulfonyl]phenyl]ethyl]amino]butyl]-4-(3-pyridinylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN   376578-67-5   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-[(trifluoromethyl)sulfonyl]phenyl]
       ethyl]amino]butyl]-4-methyl-, monohydrochloride (9CI)   (CA INDEX NAME)
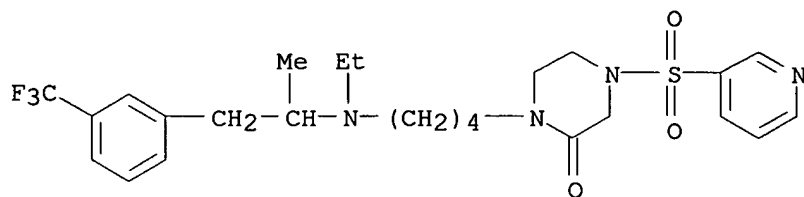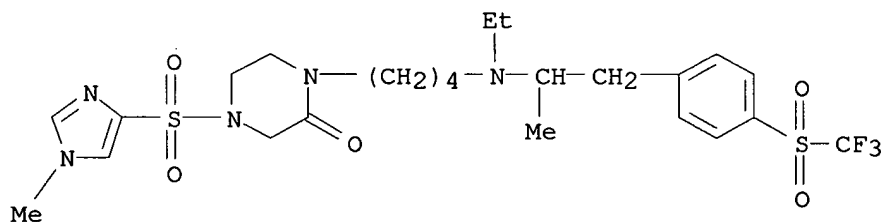

● HCl

RN   376578-69-7   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
       ]butyl]-4-(3-pyridinylsulfonyl)-, monohydrochloride (9CI)   (CA INDEX NAME)

● HCl

RN   376578-74-4   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[3-(trifluoromethyl)phenyl]ethyl]amin
       o]butyl]-4-(3-pyridinylsulfonyl)-, monohydrochloride (9CI)   (CA INDEX
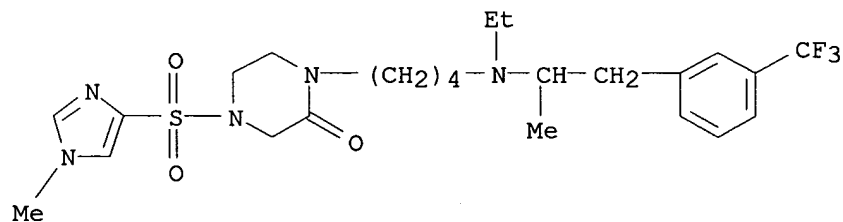   NAME)

● HCl

RN   376578-75-5   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-[(trifluoromethyl)sulfonyl]phenyl]
      ethyl]amino]butyl]-4-[(1-methyl-1H-imidazol-4-yl)sulfonyl]-,
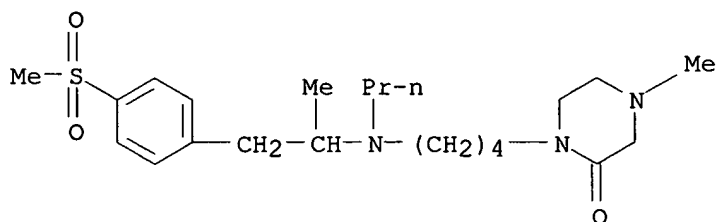   monohydrochloride (9CI)   (CA INDEX NAME)

● HCl

RN   376578-78-8   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[3-(trifluoromethyl)phenyl]ethyl]amin
      o]butyl]-4-[(1-methyl-1H-imidazol-4-yl)sulfonyl]-, dihydrochloride (9CI)
      (CA INDEX NAME)

●2 HCl

RN   376578-82-4   CAPLUS
CN   Piperazinone, 4-methyl-1-[4-[[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]p
      ropylamino]butyl]-, dihydrochloride (9CI)   (CA INDEX NAME)
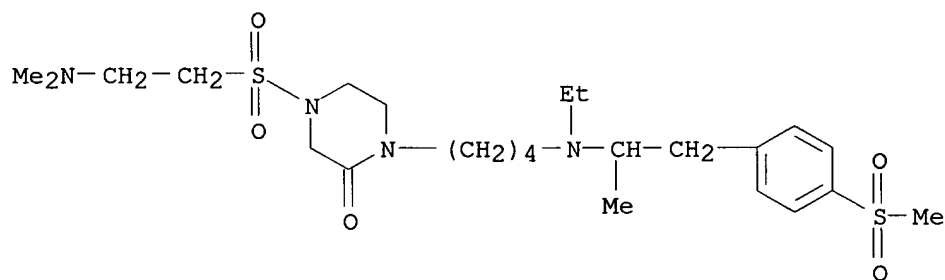
●2 HCl

RN   376579-69-0   CAPLUS
CN   Piperazinone, 4-[[2-(dimethylamino)ethyl]sulfonyl]-1-[4-[ethyl[1-methyl-2-
      [4-(methylsulfonyl)phenyl]ethyl]amino]butyl]-, mono(trifluoroacetate)
      (9CI)   (CA INDEX NAME)

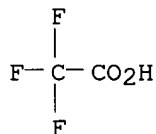   CM   1

      CRN   376579-68-9
      CMF   C24 H42 N4 O5 S2
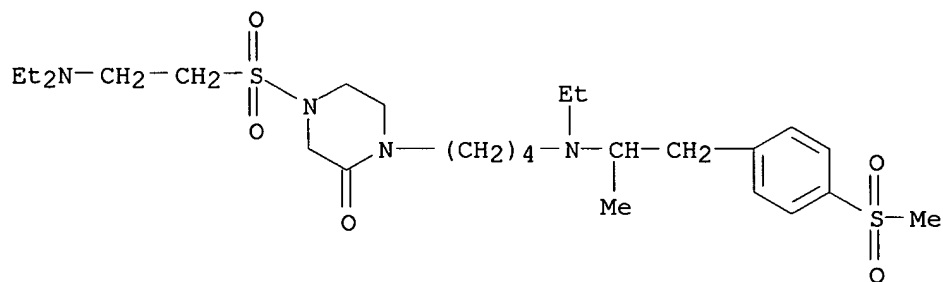

      CM   2

      CRN   76-05-1
      CMF   C2 H F3 O2

RN   376579-71-4   CAPLUS
CN   Piperazinone, 4-[[2-(diethylamino)ethyl]sulfonyl]-1-[4-[ethyl[1-methyl-2-
      [4-(methylsulfonyl)phenyl]ethyl]amino]butyl]-, mono(trifluoroacetate)
      (9CI)   (CA INDEX NAME)
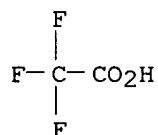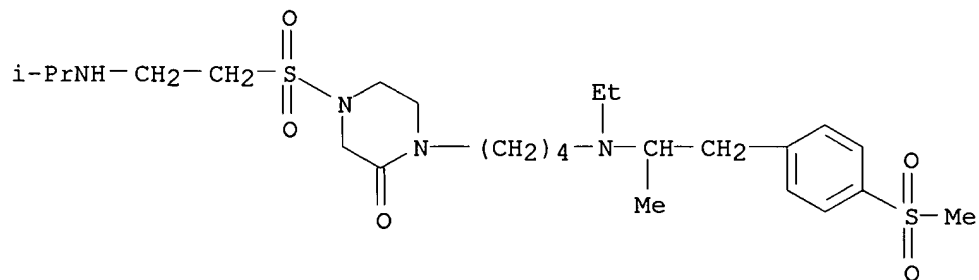
CM   1

CRN   376579-70-3
CMF   C26 H46 N4 O5 S2

$$Et_2N-CH_2-CH_2-\overset{\displaystyle O}{\underset{\displaystyle O}{\overset{\|}{\underset{\|}{S}}}}$$

[Structure: Et₂N—CH₂—CH₂—S(=O)(=O)—N(piperazinone ring with C=O)—N—(CH₂)₄—N(Et)—CH(Me)—CH₂—(phenyl)—S(=O)(=O)—Me]

CM   2

CRN   76-05-1
CMF   C2 H F3 O2

$$F-\overset{\displaystyle F}{\underset{\displaystyle F}{\overset{|}{\underset{|}{C}}}}-CO_2H$$

RN   376579-73-6   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
      ]butyl]-4-[[2-[(1-methylethyl)amino]ethyl]sulfonyl]-,
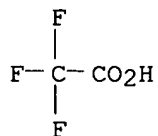   mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM   1

CRN   376579-72-5
CMF   C25 H44 N4 O5 S2

[Structure: i-PrNH—CH₂—CH₂—S(=O)(=O)—N(piperazinone ring with C=O)—N—(CH₂)₄—N(Et)—CH(Me)—CH₂—(phenyl)—S(=O)(=O)—Me]

CM   2

CRN 76-05-1
CMF C2 H F3 O2

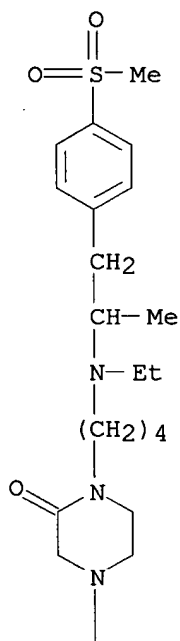$$F-\underset{\underset{F}{|}}{\overset{\overset{F}{|}}{C}}-CO_2H$$

RN 376579-75-8 CAPLUS
CN Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
]butyl]-4-[[2-(1-pyrrolidinyl)ethyl]sulfonyl]-, mono(trifluoroacetate)
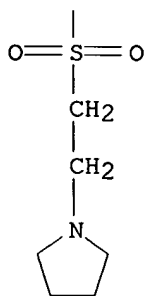(9CI) (CA INDEX NAME)

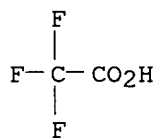CM 1

CRN 376579-74-7
CMF C26 H44 N4 O5 S2

PAGE 1-A

CM   2

CRN   76-05-1
CMF   C2 H F3 O2
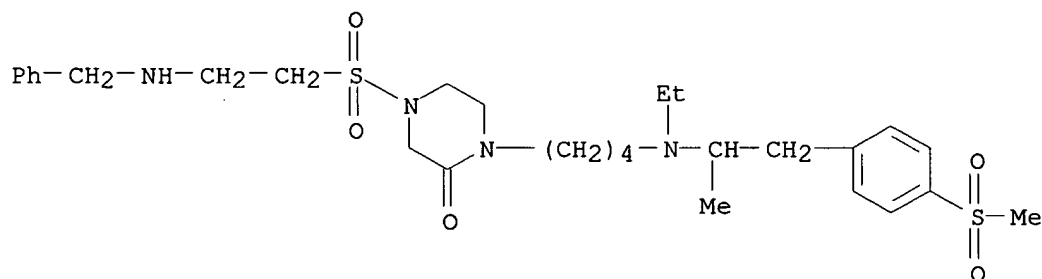
F—C—CO2H (F, F, F substituents)

RN   376579-77-0   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
      ]butyl]-4-[[2-[(phenylmethyl)amino]ethyl]sulfonyl]-,
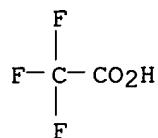   mono(trifluoroacetate) (9CI)   (CA INDEX NAME)
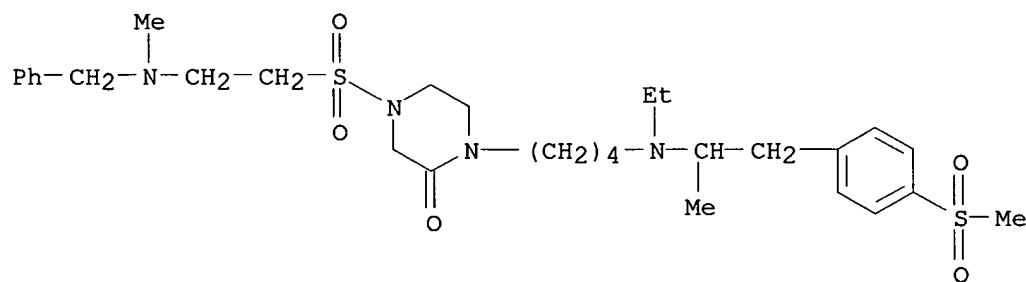
CM   1

CRN   376579-76-9
CMF   C29 H44 N4 O5 S2
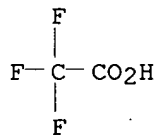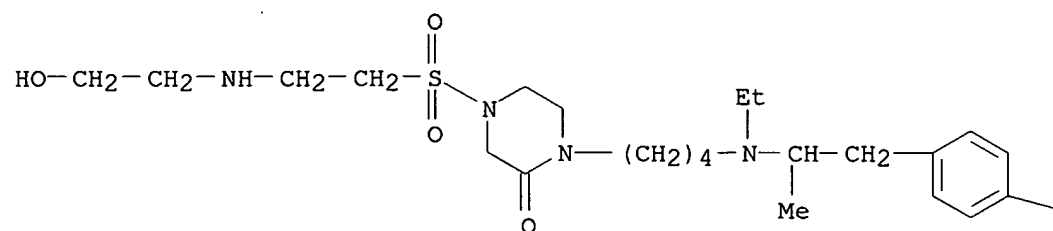
Ph—CH2—NH—CH2—CH2—S(O)(O)—N(piperazinone)—(CH2)4—N(Et)—CH(Me)—CH2—phenyl—S(O)(O)—Me

CM   2

CRN   76-05-1
CMF   C2 H F3 O2

F—C—CO2H with F substituents

F—C—CO2H with F substituents (lower)

HO—CH2—CH2—NH—CH2—CH2—S(=O)(=O)—[N-piperazinone]—N—(CH2)4—N(Et)—CH—CH2—[p-tolyl]
                                                                          |
                                                                          Me

Me—S(=O)(=O)—Me

CM   2

CRN   76-05-1
CMF   C2 H F3 O2
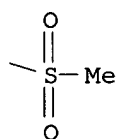
F—C(F)(F)—CO2H

RN   376579-83-8   CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
        ]butyl]-4-[[2-[(2-methoxyethyl)amino]ethyl]sulfonyl]-,
        mono(trifluoroacetate) (9CI)   (CA INDEX NAME)

CM   1

CRN   376579-82-7
CMF   C25 H44 N4 O6 S2
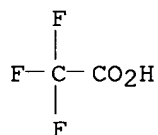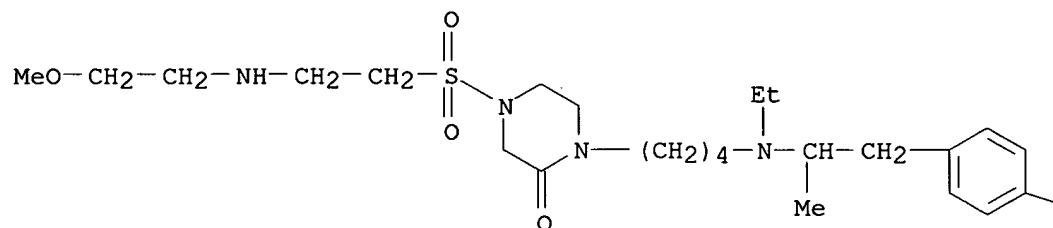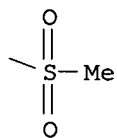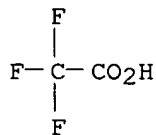
PAGE 1-A

MeO—CH2—CH2—NH—CH2—CH2—S—N(piperazine ring with sulfonyl)—(CH2)4—N(Et)—CH—CH2—(p-tolyl)

$$\text{MeO-CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-}\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle O}{\|}}{S}}\text{-N}$$

PAGE 1-B

$$\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle O}{\|}}{S}}\text{-Me}$$

CM   2

CRN   76-05-1
CMF   C2 H F3 O2

$$\text{F-}\overset{\overset{\displaystyle F}{|}}{\underset{\underset{\displaystyle F}{|}}{C}}\text{-CO}_2\text{H}$$

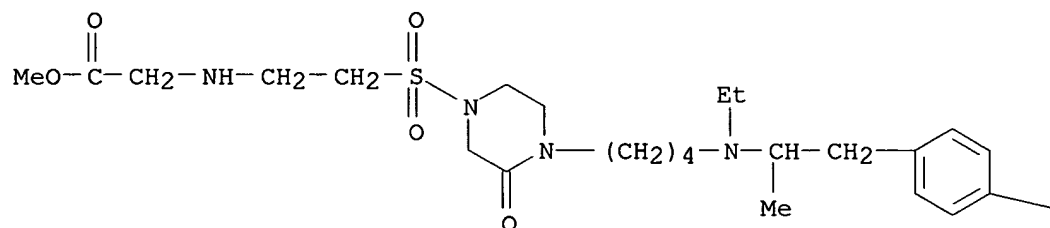RN   376579-85-0   CAPLUS
CN   Glycine, N-[2-[[4-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]ami
       no]butyl]-3-oxo-1-piperazinyl]sulfonyl]ethyl]-, methyl ester,
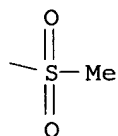   mono(trifluoroacetate) (9CI)   (CA INDEX NAME)

CM   1

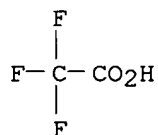CRN   376579-84-9
CMF   C25 H42 N4 O7 S2

PAGE 1-A

MeO—C(=O)—CH₂—NH—CH₂—CH₂—S(=O)₂—[piperazinone ring]—N—(CH₂)₄—N(Et)—CH(Me)—CH₂—[4-methylphenyl]

$$\text{MeO-C(=O)-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-S(O)}_2\text{-N}\langle\text{piperazinone}\rangle\text{N-(CH}_2)_4\text{-N(Et)-CH(Me)-CH}_2\text{-C}_6\text{H}_4\text{-CH}_3$$

PAGE 1-B

—S(=O)₂—Me

```
        CM    2

        CRN   76-05-1
        CMF   C2 H F3 O2
```

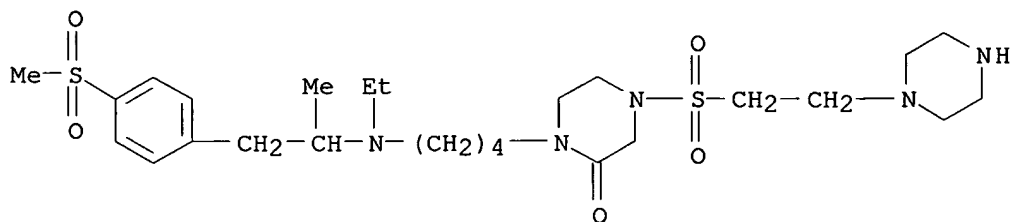F—C(F)(F)—CO₂H

```
RN    376579-87-2  CAPLUS
CN    Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
      ]butyl]-4-[[2-(1-piperazinyl)ethyl]sulfonyl]-, mono(trifluoroacetate)
      (9CI)  (CA INDEX NAME)

        CM    1

        CRN   376579-86-1
        CMF   C26 H45 N5 O5 S2
```
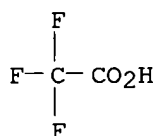
CM   2

CRN   76-05-1
CMF   C2 H F3 O2
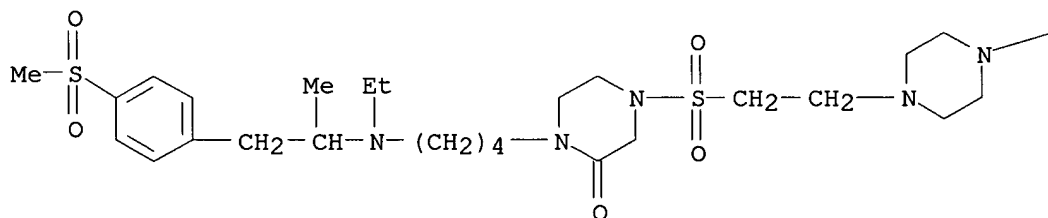

RN   376579-89-4 CAPLUS
CN   Piperazinone, 1-[4-[ethyl[1-methyl-2-[4-(methylsulfonyl)phenyl]ethyl]amino
]butyl]-4-[[2-(4-methyl-1-piperazinyl)ethyl]sulfonyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM   1

CRN   376579-88-3
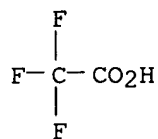CMF   C27 H47 N5 O5 S2

PAGE 1-A

PAGE 1-B

— Me

CM   2

CRN   76-05-1
CMF   C2 H F3 O2

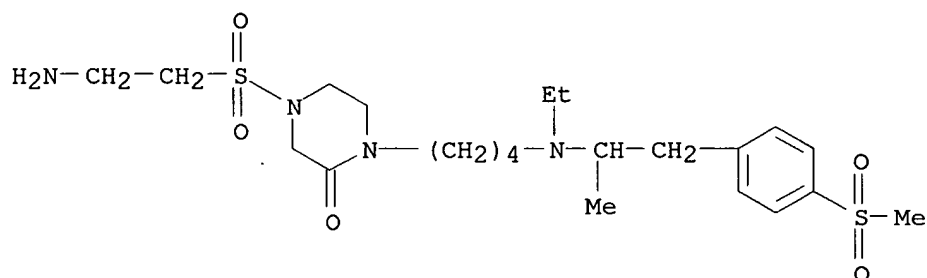F—C—CO2H (with F above, F below, bonded to C)

RN   376579-91-8 CAPLUS
CN   Piperazinone, 4-[(2-aminoethyl)sulfonyl]-1-[4-[ethyl[1-methyl-2-[4-
       (methylsulfonyl)phenyl]ethyl]amino]butyl]-, mono(trifluoroacetate) (9CI)
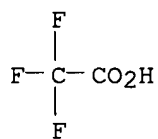   (CA INDEX NAME)

       CM   1

       CRN   376579-90-7
       CMF   C22 H38 N4 O5 S2

H2N—CH2—CH2—S(=O)(=O)—[piperazinone]—N—(CH2)4—N(Et)—CH(Me)—CH2—[phenyl]—S(=O)(=O)—Me

       CM   2

       CRN   76-05-1
       CMF   C2 H F3 O2

F—C—CO2H (with F above, F below, bonded to C)

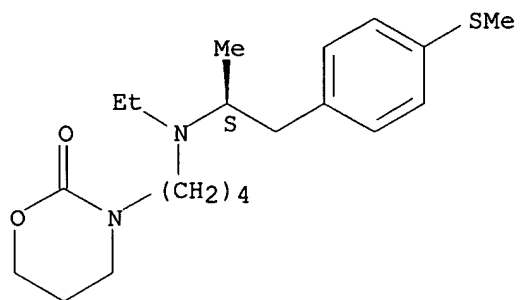IT   **376581-05-4P**
       RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
          (preparation of aminoalkyllactams as muscarinic receptor antagonists)
RN   376581-05-4 CAPLUS
CN   2H-1,3-Oxazin-2-one, 3-[4-[ethyl[(1S)-1-methyl-2-[4-
       (methylthio)phenyl]ethyl]amino]butyl]tetrahydro- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

L8   ANSWER 2 OF 2   CAPLUS   COPYRIGHT 2005 ACS on STN
AN   1977:29756   CAPLUS
DN   86:29756
TI   Studies in potential filaricides: Part VIII. Synthesis of
      1-ethyl-3-(2-dialkylaminoethyl)- and 1,3-diethyl-4-
      dialkylaminomethylhexahydropyrimidin-2-ones
AU   Singh, Harindra; Sharma, Satyavan; Iyer, R. N.; Anand, Nitya
CS   Cent. Drug Res. Inst., Lucknow, India
SO   Indian Journal of Chemistry, Section B: Organic Chemistry Including
      Medicinal Chemistry (1976), 14B(7), 528-31
      CODEN: IJSBDB; ISSN: 0376-4699
DT   Journal
LA   English
AB   The title compds. I (R = H, Me, Et, PhCH2) and II (R = Me, Et) were prepared
      Thus PhCH2NMeCH2CH2NHCH2CH2CO2Et was aminated with EtNH2 followed by reduction
      to give PhCH2NMeCH2CH2NHCH2NEtCO2Et, which was cyclized with NaOEt to give
      I (R = PhCH2). I (R = Me) reduced the microfilarial count in rats
      infected with Litomosides carinii by 90%.
IT   **61322-07-4P**
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
RN   61322-07-4 CAPLUS
CN   2(1H)-Pyrimidinone, 1-ethyltetrahydro-3-[2-[methyl(2-
      phenylethyl)amino]ethyl]- (9CI)   (CA INDEX NAME)
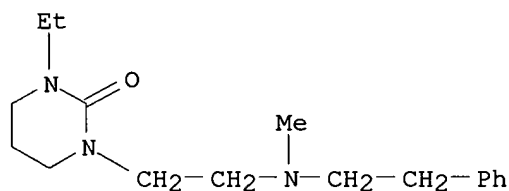
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     FILE 'REGISTRY' ENTERED AT 14:27:46 ON 25 SEP 2005
L1              STRUCTURE UPLOADED
L2          8 S L1 SSS SAM
L3        173 S L1 SSS FUL
L4              STRUCTURE UPLOADED
L5          6 S L4 SSS SAM SUB=L3
L6         90 S L4 SSS FUL SUB=L3
L7    `    83 S L3 NOT L6

     FILE 'CAPLUS' ENTERED AT 14:30:26 ON 25 SEP 2005
L8          2 S L7

     FILE 'CAOLD' ENTERED AT 14:31:00 ON 25 SEP 2005

=> s 17
L9          0 L7

=> log y
COST IN U.S. DOLLARS                         SINCE FILE     TOTAL
                                          .     ENTRY      SESSION
FULL ESTIMATED COST                             0.43       211.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE     TOTAL
                                                ENTRY      SESSION
CA SUBSCRIBER PRICE                             0.00        -1.46

STN INTERNATIONAL LOGOFF AT 14:31:11 ON 25 SEP 2005
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